An XML-Based Platform for Semantic Transformation of Numerical Programs

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ABSTRACT

We describe a simple component architecture for the development of tools for mathematically based semantic transformations of scientific software. This architecture consists of compiler-based, language-specific front- and backends for source transformation, loosely coupled with one or more language-independent "plug-in" transformation modules. The coupling mechanism between the front- and back-ends and transformation modules is provided by the XML Abstract Interface Form (XAIF). XAIF provides an abstract, language-independent representation of language constructs common in imperative languages, such as C and Fortran. We describe the use of this architecture in the construction of tools for automatic differentiation (AD) of programs written in Fortran 77 and ANSI C. The XAIF is particularly well suited for performing the source transformations needed for AD. Differentiation modules typically operate within the scope of statements or basic blocks, working at a level where procedural languages are very similar. Thus, it is possible to specify a common interface format for mathematically-based semantic transformations that need not represent the union of all languages.

KEY WORDS

source transformation, intermediate representation, automatic differentiation

1 Introduction

We describe an architecture for mathematically based semantic transformations of scientific applications. The main goal of this architecture is to allow the development of source transformation algorithms independent of the source language. The implementation of such an algorithm can be used as a "plug-in" module for a language-dependent frontend.

The mechanism connecting the components of this architecture is the XML Abstract Interface Form (XAIF). XAIF provides a language-independent representation of constructs common in imperative languages, such as C and Fortran. The main role of the XAIF is to define a layer of abstraction, so that various transformation algorithms can

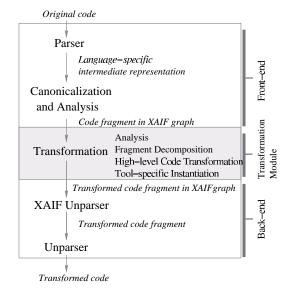


Figure 1. The Source Transformation Process.

be expressed in a language-neutral manner.

Figure 1 illustrates some of the possible steps involved in systems for mathematically-based source transformation. First, the original source code is parsed by the language-specific front-end. During the canonicalization and language-specific analysis phase, the front-end transforms the code to a semantically equivalent simplified form. In addition, high-level information may be gathered, such as the determination of the objects to be transformed or the granularity of code fragments to be transformed. The front-end collects code fragments, which may range from single statements to basic blocks to entire subroutines, and passes them to the XAIF-based transformation module. The transformation module then operates on the intermediate representation.

The module may work in several stages, including analysis to gather information about the objects to be transformed; fragment decomposition, or breaking up expressions into binary and unary operations; high-level transformations, which may specify templated algorithmic operations to be performed instead of transforming at the basic

operator level; and finally, tool-specific instantiation, such as calls to a subroutine library or inlined code. These stages are discussed in more detail in the context of automatic differentiation tools (Section 3).

The back-end (which may be part of the front-end) accepts the XAIF representing transformed fragments of the program and merges it back into the overall program structure, finally unparsing it to the original language.

We have identified the following issues in defining the interface between source transformation modules and language-specific front-ends:

- Granularity. Different types of source transformations may operate at different code granularities. For example, some of the automatic differentiation modules described in this paper transform single statements, whereas others may require basic blocks or even coarser-grained structures as input. The intermediate representation must be flexible enough to accommodate the needs of existing as well as future modules.
- Mixed strategies. The intermediate representation must enable the application of different transformation strategies on different portions of the code.
- Efficient intermediate code analysis and transformation. Most AD algorithms for generating robust and
 efficient derivative code use elements from data flow
 analysis and standard graph algorithms developed for
 a variety of closely related problems including modern
 compiler technology [1, 2] and graph algorithms [3].
 The XAIF should enable reuse of most of the available
 algorithms, thus avoiding unnecessary "re-inventions
 of the wheel".
- Abstraction away from language specifics. Our goal is not to define an abstract intermediate representation that comprises the union of all supported languages; instead, we must identify the subset of features occuring in portions of source code that correspond to mathematical operations. We provide abstractions of common constructs and rely on the front-end to provide mappings to and from language-specific constructs. Keeping the representation as simple as possible not only makes tool development easier, but it may also make it possible to perform optimizations that would be infeasible if the representation is complicated by language-dependent details.
- Extensibility. The intermediate format should be extensible in order to support various modules, which may define or require new features.
- *Syntax*. The syntax should be simple, yet flexible enough to represent program structure at multiple levels. Furthermore, the syntax should be easy to parse and validate.

The rest of this paper is organized as follows. Section 2 contains an introductory overview of automatic differentiation. Section 3 discusses the software architecture used in the construction of tools for automatic differentiation. Section 4 gives a brief overview of XAIF features and design. Section 5 presents the use of the XAIF in the automatic differentiation of a simple example. Section 6 summarizes our contributions.

2 Automatic Differentiation

Automatic differentiation (AD) transforms numerical programs for evaluating vector functions $f: x \in \mathbb{R}^n \mapsto y \in \mathbb{R}^m$ with n inputs and m outputs into new programs that compute derivatives of (some of) the outputs with respect to (some of) the inputs. Dating back to 1964 [4], AD has been developed over the years [5, 6, 7] to become an established tool for performing a well-defined set of semantic transformations on numerical programs. Most of the mathematical theory behind AD algorithms is covered in [8]. The research leading to this paper has been motivated by the large number of general source transformation issues related to AD.

Without going into much mathematical detail, let us briefly introduce the main concepts behind AD. For a given set of input values, the steps performed by the program can be represented as a directed acyclic computational graph. The structure of this graph can be determined at compile time for control-flow-independent parts of the program, such as single statements or basic blocks [9]. AD exploits the fact that expressions for the local partial derivatives with respect to the operands can be generated for all elementary arithmetic operations (+,-,*,/) and intrinsic functions (\sin, \exp, \ldots). For example, it is well known that $\frac{\partial (a*b)}{\partial a} = b, \frac{\partial (a*b)}{\partial b} = a, \frac{\partial (t+s)}{\partial t} = 1, \frac{\partial (x-y)}{\partial y} = -1, \frac{\partial \cos(x)}{\partial x} = -\sin(x), \frac{\partial \exp(w)}{\partial w} = \exp(w)$, etc. .

The forward and reverse modes of AD generate expressions for all local partial derivatives and exploit the chain rule to propagate Jacobian times matrix (forward-mode) or Jacobian transposed times matrix (reverse-mode) products. The Jacobian matrix contains the partial derivatives of a subset of the outputs (the dependent variables) with respect to a subset of the inputs (the independent variables). Intermediate variables that depend on some independent variable, and upon which some dependent variable depends, are called *active*.

Forward-mode AD transforms the original code so that one or more directional derivatives are propagated forward for all active variables a. These values are equal to the inner product of the gradient of a with respect to the n independent variables and some *direction* vector. Thus, the whole Jacobian can be accumulated by letting these directions range over the Cartesian basis vectors in \mathbb{R}^n .

In reverse mode the semantics of the program is changed to propagate adjoints backward for all active variables. The adjoint of an active intermediate variable a is

equal to the inner product of some *normal* vector times the vector containing the partial derivatives of the m dependent variables with respect to a. Consequently, the whole Jacobian can be accumulated by letting these normals range over the Cartesian basis vectors in \mathbb{R}^m .

Forward and reverse modes are two fundamental representatives out of a large set of AD-related semantic transformation of numerical programs. Optimal statement and basic-block level pre-accumulation techniques [10], higher-order derivatives [11], and derivatives of programs exploiting parallelism [12], to name only a few more advanced AD techniques, require highly sophisticated and extremely flexible source transformation platforms. The aim of the XAIF is to provide a quasi standard for the fast implementation of well-known and new AD algorithms and other mathematically-based semantic transformations, and thus help make them applicable a large variety of realworld problems implemented as numerical programs written in arbitrary imperative programming languages.

3 Construction of Tools for Automatic Differentiation

AD systems such as ADIFOR (for Fortran code) [13] and ADIC (for C code) [14] use compiler techniques to augment source code with statements for computing derivatives. One motivation for this source transformation approach is that it enables the tool to perform analyses, possibly interprocedural, at compile time to reduce the cost of computing derivatives. This provides a performance advantage over AD tools that use operator overloading to propagate derivatives. Robust source transformation tools are, however, considerably more difficult to implement because they require a language-specific infrastructure for parsing, analysis, canonicalization, optimization, and unparsing.

Early AD tools have been built in a monolithic fashion, without regard for reusing parts with common functionality. It is possible, however, to decouple the development of algorithms that exploit the chain rule from the infrastructure that deals with the language and the user interface. This decoupling leads to a software architecture for semantic transformation tools, in which loosely connected components communicate through an abstract interface. Defining a language-independent interface suitable for tools for automatic differentiation and similar types of semantic transformation is simpler than the general case of source transformation, since the transformations occur at a level where most imperative languages are semantically equivalent.

Figure 2 illustrates the roles of the front and backends and transformation components in the semantic transformation process. The front-end is responsible for several tasks:

 Parsing the source code and building the languagedependent intermediate representation.

- Canonicalizing the language-dependent intermediate representation. In the code canonicalization stage, code is rewritten into a standard form. For example, function calls appearing within conditional tests are hoisted into assignments to new temporary variables.
- Performing any necessary analyses, for example, determining which variables are active and thus need to have derivative objects associated with them. During this stage, the ADIFOR preprocessor applies interprocedural analysis techniques to determine which variables in a code fragment are active.
- Producing the language-independent XAIF representation. Portions of the language-dependent internal representation are translated into XAIF.
- Unparsing the transformed XAIF code back into the source language. Derivative code is generated for each assignment statement containing an active variable, and derivative objects are allocated.

The plug-in AD modules are usually responsible for three tasks:

- Defining the shape and size of new (derivative) objects. The module may declare one or more derivative objects to be associated with each active variable. The XAIF interface also provides a mechanism for declaring temporary variables.
- Augmenting statements involving active variables with derivative computations corresponding to the differentiation method.
- Specifying variable type conversions (for active variables).

In general, a series of transformations can be applied to the intermediate representation by one or more transformation modules.

4 XAIF Overview

The XAIF defines a canonical set of constructs that represent the original program in a language-independent fashion. A major challenge in defining the source transformation component interface is to identify common features in imperative languages such as C and Fortran. Representing these commonalities in an abstract fashion makes it possible to apply the same transformation algorithm in all supported languages.

The precursor to the XAIF, generically referred to as the Automatic differentiation Intermediate Format (AIF) [15], is a tree-based representation, with no support for call graph or control flow information. Furthermore, the different language-dependent front-ends that generate the AIF use different syntax. For example, the notation used by ADIFOR is based on functional programming, so the intermediate representation is generated in the functional

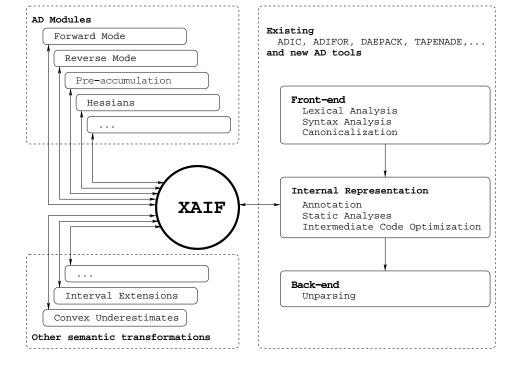


Figure 2. Role of XAIF

programming language Scheme. ADIC uses a custom textbased representation, with additional parsing and unparsing support. While the intermediate representation generated by both tools is semantically equivalent, transformation modules must translate between formats in order to operate with both front-ends. Our experience indicates that it is hard to ensure that all tool developers conform to the same custom-defined syntax for the intermediate form. While allowing different syntax for the intermediate representation provides flexibility for the language-dependent front-ends, the lack of a shared syntax makes using the same plug-in module with both tools problematic. A translator can be used to convert between formats; however, this solution is not scalable and complicates validation. Furthermore, the implementation of the module must be updated each time a tool introduces different syntax (without modifying the semantics).

XAIF decouples the language-specific portions of the source transformation process from the languageindependent transformation algorithms. This approach provides several benefits:

- Language independence. XAIF is an encapsulation of the operations relevant to semantic transformation of scientific software. We want to avoid trying to find an abstract representation of non-AD-specific features of each language, such as side-effects and pointer tracking in C and C++.
- *Tool independence*. We want to be able to write each transformation module once and have it work with multiple tools without modification. For example,

we have developed a second-order derivative (Hessian) module that works with both ADIC and ADIFOR; it can also be plugged into any tool that meets the XAIF specifications. Widely available validating XML parsers provide further flexibility in parsing and generating the intermediate form.

- Implementation independence. The language-specific
 front-end does not need to know the details of how
 the derivative augmentation is performed or what the
 derivative objects look like. Conversely, the AD module does not need to know how variables are declared
 or how derivative objects are associated with active
 variables. The components of the AD system can be
 changed, either subtly or radically, without requiring
 that other system components be modified.
- Rapid development of new algorithms. The XAIF
 component architecture provides a "workbench" for
 easily and rapidly implementing new algorithms. This
 capability has proved valuable with the Hessian module, where the most efficient algorithm was not known
 a priori. A number of different algorithms were
 quickly implemented for comparison. Also, this enabled straightforward experimentation with mixing
 different differentiation modes, which has produced
 more efficient derivative code in some cases.

We have selected XML [16, 17] for the abstract intermediate representation in part to remedy this problem. XML offers the following benefits in the context of AD tool development:

- Standard interface. XML is a W3C-endorsed standard for document markup that is flexible enough to provide the infrastructure for component coupling described in this paper.
- Widely available validating parsers. When creating
 new modules, developers do not need to implement
 a parser for processing the intermediate format from
 scratch; the general availability of XML parsers has
 simplified the task of parsing and producing XAIF.
 We implement the semantics of the XAIF by defining
 a schema, which can be used by a validating parser
 to ensure that the intermediate representation passed
 between components is valid.
- Extensibility. The X in XML stands for extensible. XML is a meta-markup language. It doesn't have a fixed set of tags and elements; instead, XML enables users to define needed elements and the relationships between them. The language can be extended and adapted to meet different needs, some of which cannot be anticipated at the time a tool is developed. The XAIF schema allows future extensions to accommodate new types of transformation such as the generation of interval extensions [18] or convex underestimates [19].

The XAIF representation consists of a series of nested graphs. All graph elements are of type GraphType, whose definition is similar to the XGMML notion of a graph [20]. All elements of GraphType contain at least one element of VertexType and zero or more elements of EdgeType. All elements of VertexType have identifiers that are unique within the parent graph element. Edges have unique identifiers, as well as key references to source and target vertices. At the highest level, the program is represented by a CallGraph element, whose children are vertices corresponding to subroutines and edges signifying subroutine calls. Each CallGraph vertex contains a ControlFlowGraph element, whose vertices and edges represent the control flow of the program. A ControlFlowVertex can contain a BasicBlockGraph, a ForLoopGraph, an IfConditionGraph, or, in general, any statement that affects the flow of control in the computation. At the bottom of the hierarchy are ExpressionGraph and symbol reference elements. SymbolTable elements can be children of any graph element and contain symbol information for the corresponding scope.

Additional information on the XAIF, including the schema definition and an example, is available at www.mcs.anl.gov/xaif.

5 Example

In this section we show how the XAIF is used in the automatic differentiation of the C code shown in Figure 3. The complete example, including the XAIF for the original

and transformed source code, is available at the XAIF web page.

```
void head(double x, double y) {
  int i;
  for (i=1;i<10;i++) {
    compute(x,y);
    if (y<0) exit;
  }
}

void compute(double x, double y) {
  double h;
  h=exp(x*x*x);
  y=sin(h*x);
}</pre>
```

Figure 3. Original source code.

5.1 XAIF of Original Program

In XAIF, a program is represented as a hierarchy of directed graphs, as shown in Figure 4. The call graph consists of two vertices representing the two subroutines head and compute (see Figure 5). The call of compute inside head is represented by the edge connecting these vertices.

The control flow graph of head (Figure 6) contains three vertices in addition to the standard entry and exit vertices. If the for-loop condition is satisfied, the loop body gets executed. Otherwise, the program is continued with the first statement following the loop. In this example no statement follows the loop, which results in an edge leading into the exit vertex.

The first statement inside the loop body is the call of compute followed by an if-statement. Depending on the value of the test, the loop is exited or the next statement in the loop body is executed. As the if-statement happens to be the last statement of the loop body, this is equivalent to jumping back to the head of the loop.

The control flow inside compute is straightforward. It consists of a single basic block in addition to entry and exit. After canonicalization (performed by the

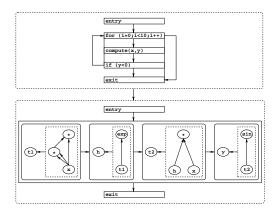


Figure 4. XAIF Graph Hierarchy

Figure 5. Call graph XAIF representation.

```
<xaif:ControlFlowGraph>
 <xaif:ControlFlowGraphProperties>
 </xaif:ControlFlowGraphProperties>
 <xaif:SymbolTable>
 </xaif:SymbolTable>
 <xaif:ControlFlowVertex id="0" name="Entry"/>
 <xaif:ControlFlowVertex id="1" name="ForLoop">...</xaif:ControlFlowVertex>
 <xaif:ControlFlowVertex id="2" name="BasicBlock">...</xaif:ControlFlowVertex>
 <xaif:ControlFlowVertex id="3" name="If">...</xaif:ControlFlowVertex>
 <xaif:ControlFlowVertex id="4" name="Exit"/>
 <xaif:ControlFlowEdge id="0" source="0" target="1"/>
 <xaif:ControlFlowEdge id="1" source="1" target="4"/>
 <xaif:ControlFlowEdge id="2" source="1" target="2"/>
 <xaif:ControlFlowEdge id="3" source="2" target="3"/>
 <xaif:ControlFlowEdge id="4" source="3" target="1"/>
 <xaif:ControlFlowEdge id="5" source="3" target="4"/>
</xaif:ControlFlowGraph>
```

Figure 6. Control flow graph XAIF representation.

front-end), the basic block contains four assignment statements, which are represented by the four vertices of the BasicBlockGraph element shown in Figure 7.

Each AssignmentStatementGraph consists of a variable reference representing the left-hand side and some expression DAG representing the right-hand side, as illustrated in Figure 8.

The minimal vertices in the expression DAGs represent variable references. All other vertices are arithmetic operations or function calls. The value associated with the maximal vertex is assigned to the variable referenced on the left-hand side. Intermediate results are labeled $v1, \ldots, v5$.

5.2 XAIF of Transformed Program

In this section we describe the result of transforming the original program semantically according to a two-step AD

algorithm:

- 1. Derivative code for computing the local Jacobian of the basic block in compute is generated. Since in this simple example there are just one independent x and one dependent y variable, the local Jacobian contains only one element $\partial y/\partial x$, which is the derivative of y with respect to x.
- 2. As noted in Section 2, derivative code generated according to the rules of forward-mode AD computes directional derivatives of the dependent with respect to the independent variables, that is, Jacobian matrix times vector products. In the example, this simplifies to a weighted derivative, namely, the product of ∂y/∂x and some scalar weight ad_x. The semantics of the program is changed in order to compute this value.

```
<xaif:BasicBlockGraph>
 <xaif:BasicBlockGraphProperties>
   <xaif:Property id="0" name="inloop" value="no"/>
 </xaif:BasicBlockGraphProperties>
 <!-- t.1 = x*x*x; -->
 <xaif:BasicBlockVertex id="0" name="AssignmentStatementGraph">
 </raif:BasicBlockVertex>
 <!-- h = \exp(t1); -->
 <xaif:BasicBlockVertex id="1" name="AssignmentStatementGraph">
  </xaif:BasicBlockVertex>
 <!-- +2 = h*x; -->
 <xaif:BasicBlockVertex id="2" name="AssignmentStatementGraph">
 </xaif:BasicBlockVertex>
 <!-- y = sin(t2); -->
 <xaif:BasicBlockVertex id="3" name="AssignmentStatementGraph">
 </xaif:BasicBlockVertex>
 <!-- data flow -->
  <xaif:BasicBlockEdge id="0" source="0" target="1"/>
  <xaif:BasicBlockEdge id="1" source="1" target="2"/>
  <xaif:BasicBlockEdge id="2" source="2" target="3"/>
</xaif:BasicBlockGraph>
```

Figure 7. Basic block graph XAIF representation.

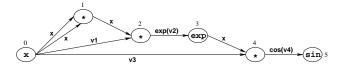


Figure 9. Linearized Computational Graph

Building on the AD basics introduced in section 2 and referencing relevant literature, we briefly discuss a method for generating optimal derivative code for the local Jacobian of compute. The main elements of the corresponding XAIF representation are presented in the context of the XAIF of the forward-mode AD transformed code.

The computational graph of the basic block is shown in Figure 9. Expressions for the local partial derivatives are attached to the edges. Given a value for x, one can evaluate these expressions during a single evaluation of the basic block in parallel with the actual function value y itself. This results in a linearized version of the computational graph. As shown in [21], the value of derivative $\partial y/\partial x$ at the current argument can be accumulated by eliminating the p intermediate vertices in the linearized computational graph (in our example, p=4). The order in which this is done determines the number of scalar floating-point operations required for this process. Minimizing this value over the p! different elimination orderings is conjectured to be an NP-complete combinatorial optimization problem [22, 21].

A deterministic algorithm for gradients with singleread intermediate variables (such as the graph in our exam-

```
void compute_ad(double x, double ad_x,
                double y, double ad_y) {
 double h;
 double t1, t2;
 double _dy_dx_t1,_dy_dx_t2,_dy_dx_t3,_dy_dx_t4;
 double dv dx;
 t.1=x*x*x;
 h=exp(t1);
 t2=h*x;
 y=sin(t2);
 _dy_dx_t1 = (x+x)*x+x*x
 _dy_dx_t2 = exp(t1)
  _dy_dx_t3 = _dy_dx_t1*_dy_dx_t2*x+h
 _{dy_{dx_t4}} = cos(t2)
 _{dy_dx} = _{dy_dx_t3*_dy_dx_t4}
 ad_y = _dy_dx * ad_x
```

Figure 10. Derivative code for the compute function.

ple) is discussed in [23]. It leads to the derivative code for compute shown in Figure 10.

The computation of _dy_dx_t1 corresponds to the elimination of vertex 1 in the linearized computational graph. Vertices 2 and 3 are eliminated by computing _dy_dx_t3. Finally, the elimination of vertex 4 leads to _dy_dx, which represents the pre-accumulated value of $\partial y/\partial x$. The subroutine itself is transformed into a semantically different version compute_ad with inputs x and ad_x and outputs y and ad_y. It is straightforward to verify that for a given argument x and a derivative weight

```
<!-- t2 = h*x; -->
<xaif:BasicBlockVertex id="2" name="AssignmentStatementGraph">
  <xaif:AssignmentStatementGraph>
    <xaif:VariableReferenceVertex id="0" symbolId="1 4"/>
    <xaif:AssignmentRHSVertex id="1">
      <xaif:ExpressionGraph>
        <xaif:VariableReferenceVertex id="0" symbolId="1_3"/>
        <xaif:VariableReferenceVertex id="1" symbolId="1_1"/>
        <xaif:BinaryExpressionVertex id="2" name="Multiply"/>
        <xaif:ExpressionEdge id="0" source="0" target="2"/>
<xaif:ExpressionEdge id="1" source="1" target="2"/>
      </xaif:ExpressionGraph>
    </xaif:AssignmentRHSVertex>
    <xaif:AssignmentStatementEdge id="0" source="1" target="0"/>
  </xaif:AssignmentStatementGraph>
</xaif:BasicBlockVertex>
<!-- y = sin(t2); -->
<xaif:BasicBlockVertex id="3" name="AssignmentStatementGraph">
  <xaif:AssignmentStatementGraph>
    <xaif:StatementProperties>
    </xaif:StatementProperties>
    <xaif:VariableReferenceVertex id="0" symbolId="1_5"/>
    <xaif:AssignmentRHSVertex id="1">
      <xaif:ExpressionGraph>
        <xaif:SubroutineCallExpressionVertex id="0" symbolId="exp">
          <xaif:SubroutineArgument;</pre>
             <xaif:VariableReference symbolId="1_4"/>
          </xaif:SubroutineArgument>
        </xaif:SubroutineCallExpressionVertex
      </xaif:ExpressionGraph>
    </xaif:AssignmentRHSVertex>
    <xaif:AssignmentStatementEdge id="0" source="1" target="0"/>
  </xaif:AssignmentStatementGraph>
</xaif:BasicBlockVertex>
```

Figure 8. Assignment statement graph XAIF representation.

Figure 11. Derivative code for the head function.

ad_x, compute_ad computes both the function value y and ad_y—the directional derivative of y with respect to x in direction ad_x. This is what we expect from a forward-mode AD-transformed derivative code. The XAIF of compute_ad is analogous to the one for the original routine, with a basic block containing additional assignments and several new entries in the symbol table and argument list.

The forward-mode AD version of the top-level routine head is shown in Figure 11. The control flow remains unchanged: head_ad calls compute_ad to compute both y and ad_y for given x and ad_x. Again, the XAIF is analogous to the one for the head subroutine with the necessary changes or additions made to the symbol table, argument list, and call to compute. The XAIF of the entire derivative code can be found at www.mcs.anl.gov/xaif.

6 Summary

We have presented a simple component architecture for the development of semantic transformation tools based on the XML Abstract Interface Form, an abstract representation of the common features in imperative languages. XAIF decouples the language-specific front-end, which performs parsing, analysis, and unparsing functions, from languageindependent transformations. XAIF provides the interface that enables the rapid development of plug-in semantic transformation modules that interoperate with multiple language-specific front-ends. We have demonstrated the utility of this architecture in the context of automatic differentiation, and illustrated the use of the XAIF in a forward-mode differentiation module. Although our experience to date is focused on automatic differentiation, we believe the XAIF architecture will naturally accommodate other mathematically-based transformations, such as interval computations.

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